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*Publication date:*  
2010

*Document Version*  
Publisher's PDF, also known as Version of record

[Link back to DTU Orbit](#)

*Citation (APA):*  
Yunus, N. A. (Author), Manan, Z. A. (Author), Hashim, H. (Author), & Gani, R. (Author). (2010). Design of Feasible Blends of Gasoline and Biofuels using a Systematic Computer Aided Technique. Sound/Visual production (digital)

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# DESIGN OF FEASIBLE BLENDS OF GASOLINE AND BIOFUELS USING A SYSTEMATIC COMPUTER AIDED TECHNIQUE

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Haslenda Hashim and Rafiqul Gani

BY:

NOR ALAFIZA YUNUS

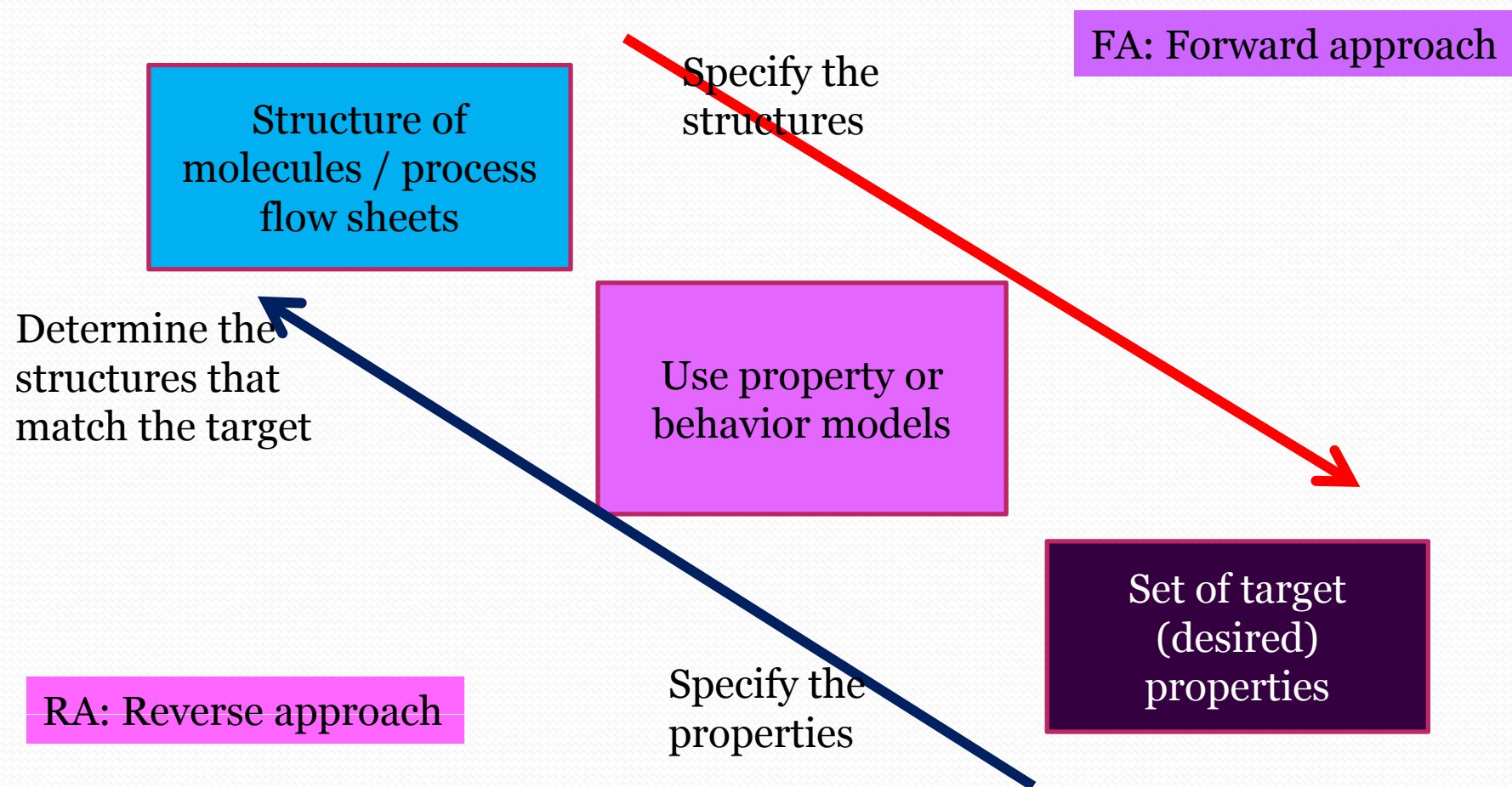
5th PSE ASIA, July 25 - 28, 2010 Singapore

# Outline

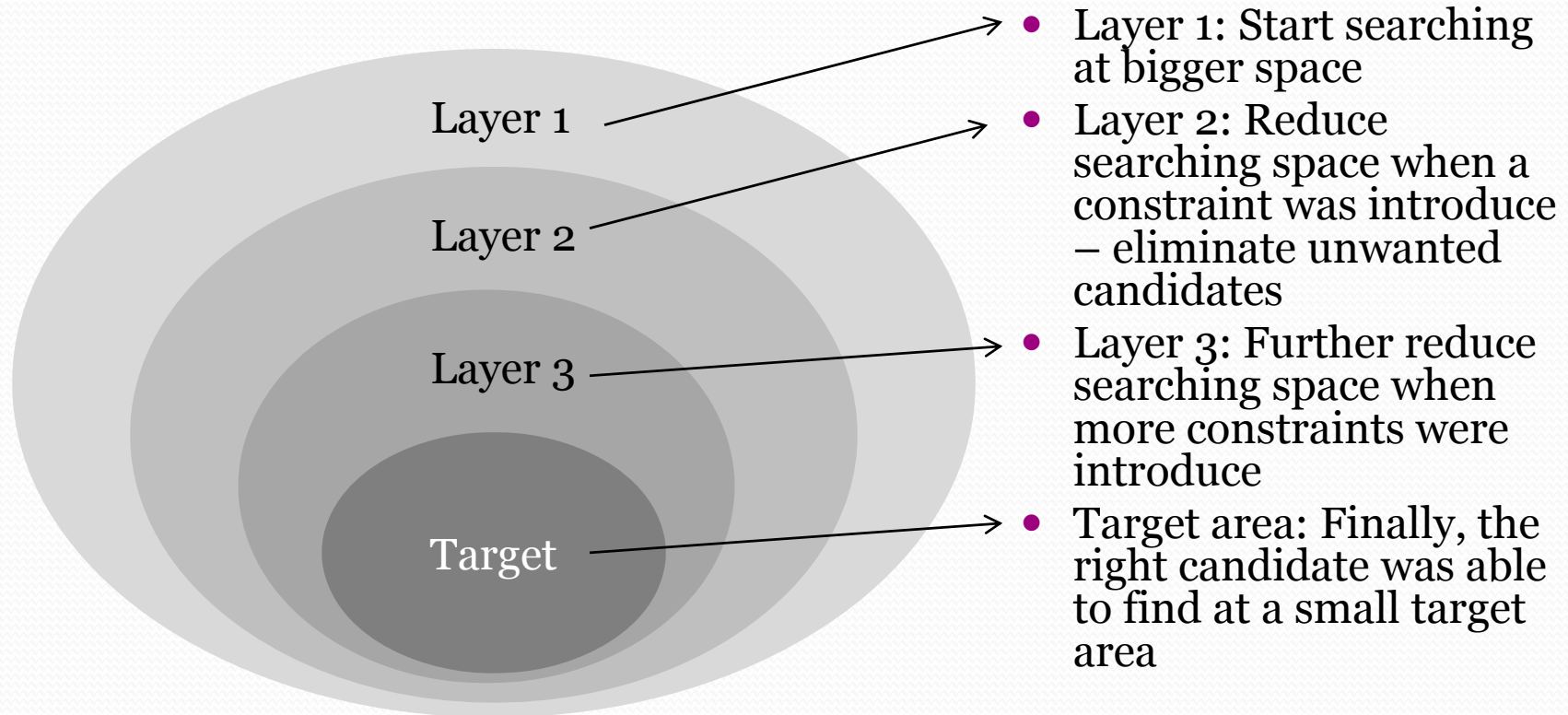
- Introduction
- Motivation
- Objective
- Methodology
- Results
- Future work

# Introduction

## Chemical Product Design



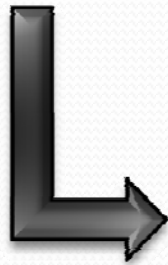
# Introduction



# Motivation

## Gasoline

- ❖ Shortage of fossil supply
- ❖ Emit large amount of CO<sub>2</sub>



Gasoline



Bio- fuel



Prolong the gasoline  
supply &  
Reduce CO<sub>2</sub>  
emission



Method of  
blending



Computer aided  
method – GAMS &  
ICAS software

# Objective

To find a set of feasible blend of gasoline and bio-fuel which are could reduce fossil fuel consumption using a systematic computer aided approach

# Methodology

Step 1

Identify target properties and target values

Step 2

Identify properties model

Step 3

Identify the possible blend mixture

Step 4

Generate the possible blend candidates

Step 5

Validate the model

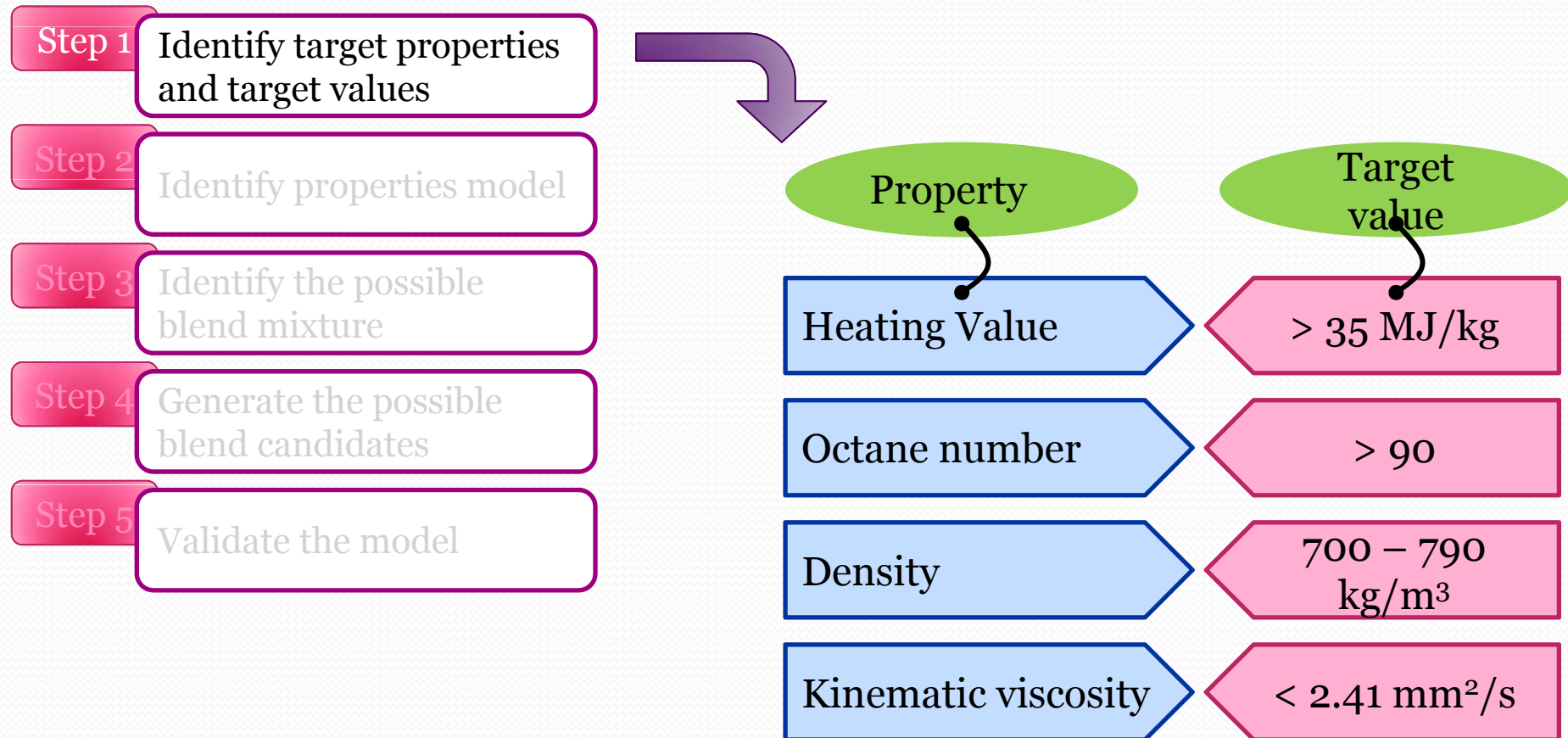


# Methodology

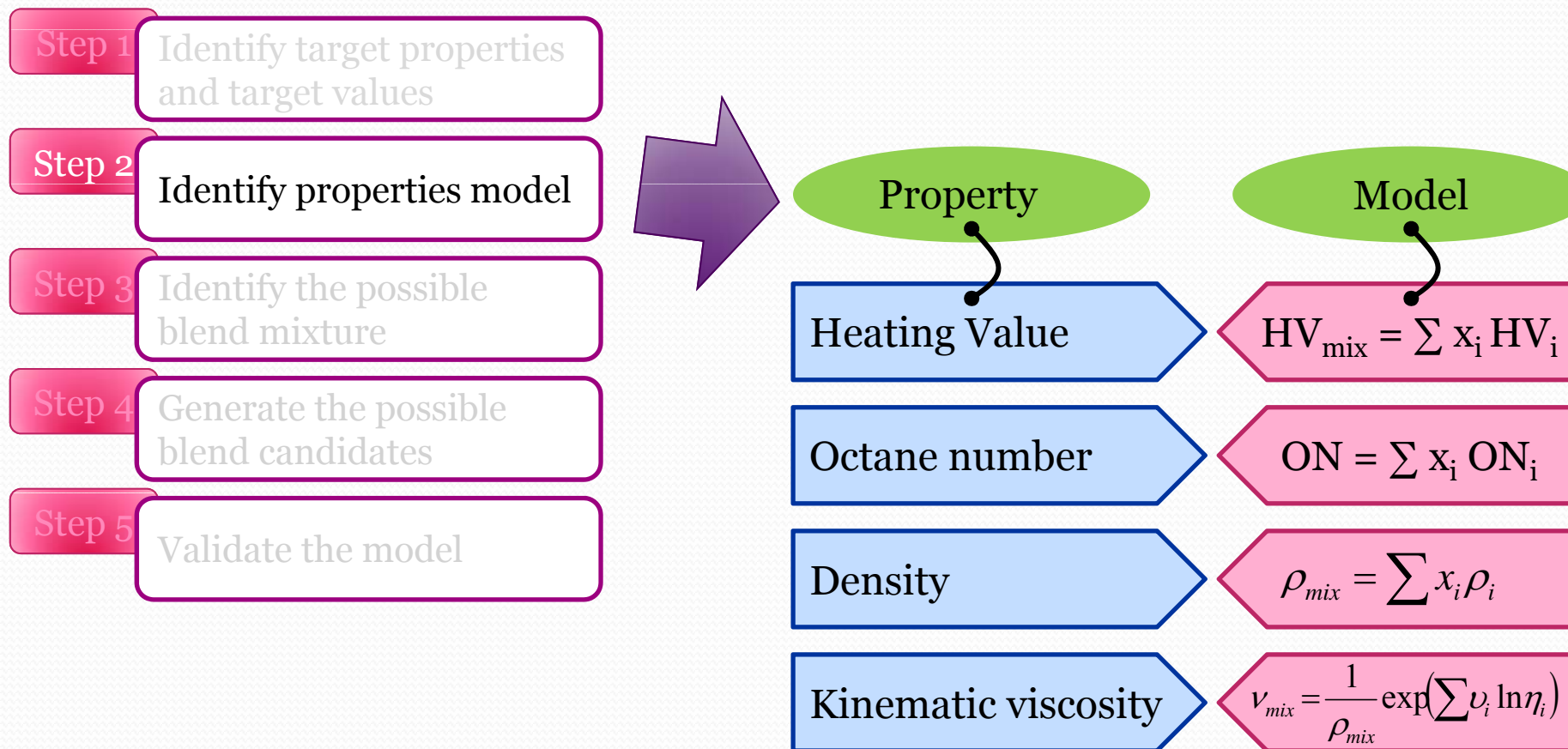
step	Task	Method & tools	Output
1	Identify the important target property	Literature (journals) Blending guideline	List of target properties
	Set the target value for each target property	Literature (journals), Blending regulation Existing product	List of constraints
2	Identify pure and mixture property model	Literature, calculated directly from chemical structure	Pure property models Mixture property models
3	Identify the feasible mixture	ICAS	List of feasible blend compositions
4	Generate the possible mixture candidates	GAMS	List of several possible mixture candidates
5	Model validation	Experiment	Experimental data

ICAS: Integrated Computer Aided System

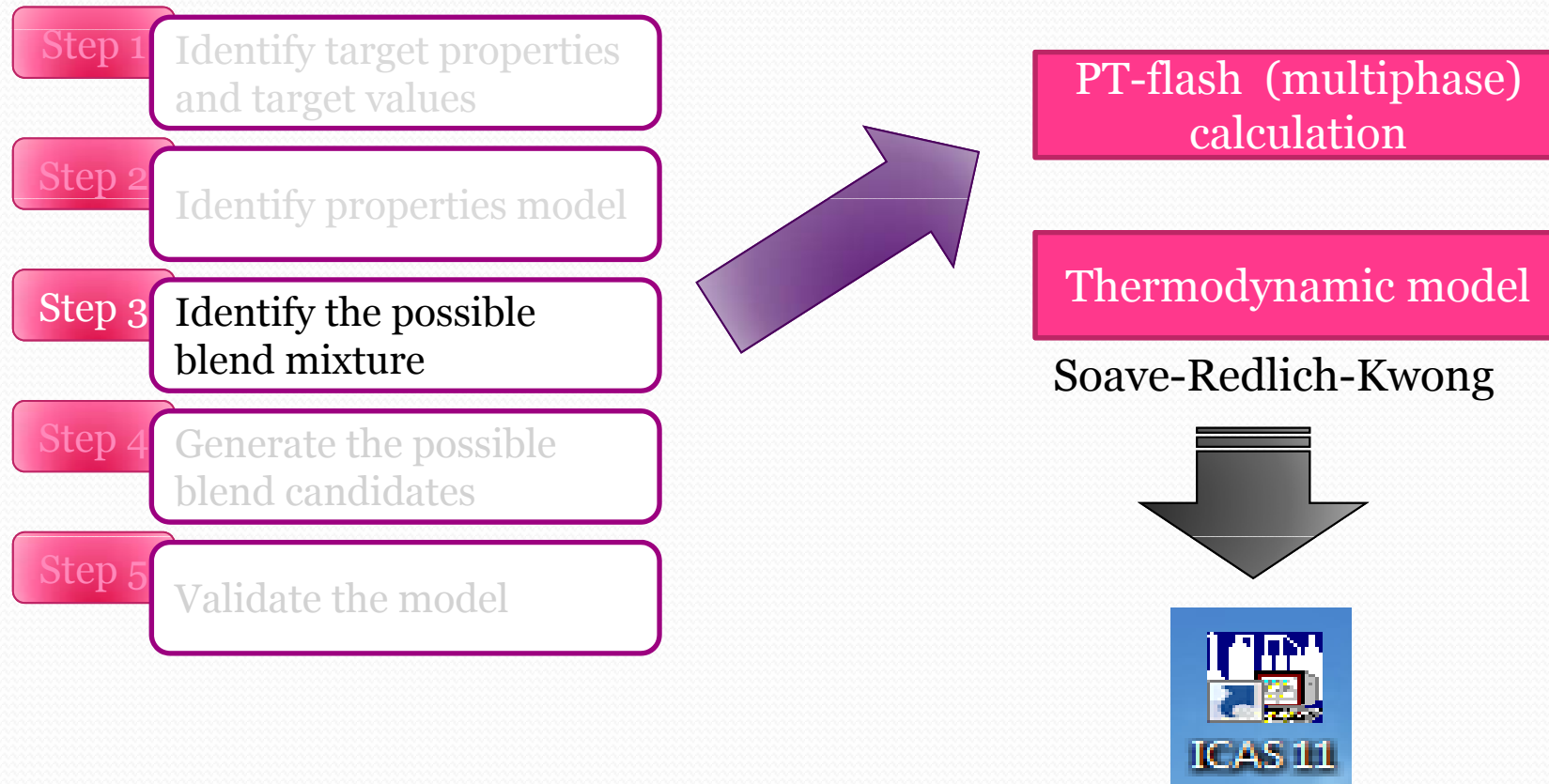
# Methodology



# Methodology



# Methodology



# Methodology

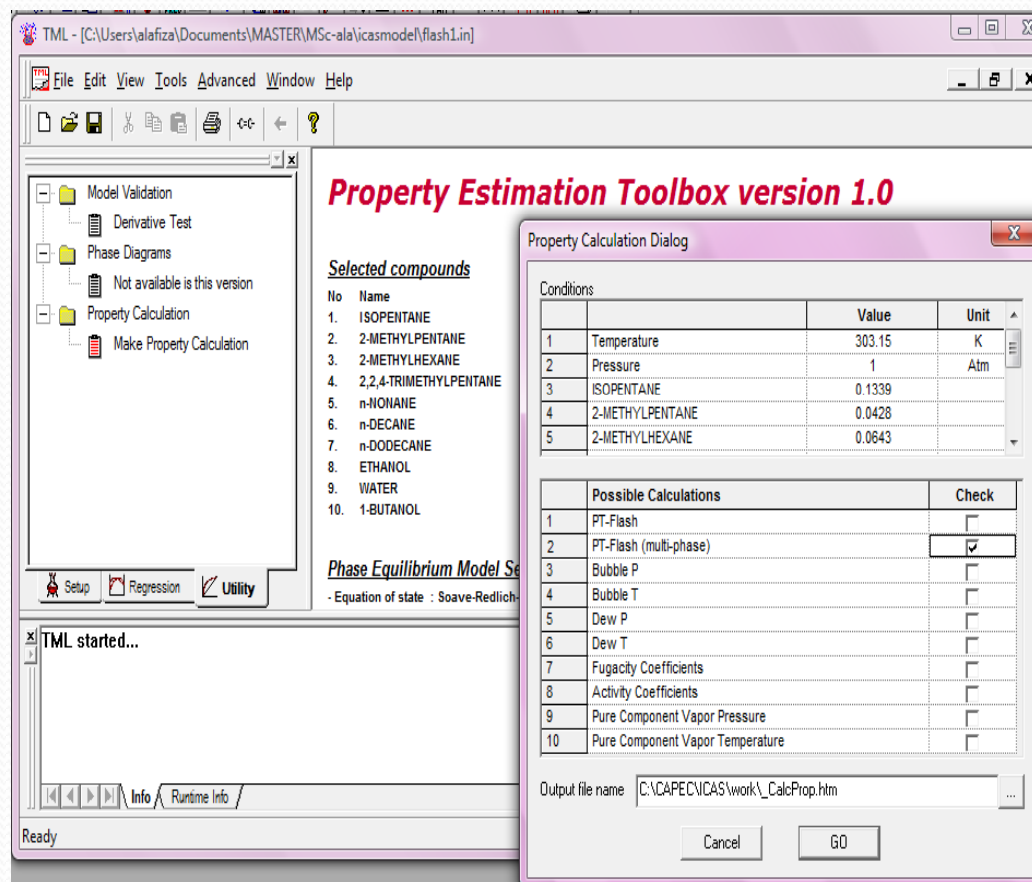
Step 1 Identify target properties and target values

Step 2 Identify properties model

Step 3 Identify the possible blend mixture

Step 4 Generate the possible blend candidates

Step 5 Validate the model



# Methodology

Step 1 Identify target properties and target values

Step 2 Identify properties model

Step 3 Identify the possible blend mixture

Step 4 Generate the possible blend candidates

Step 5 Validate the model

TML - [C:\CAPEC\UCAS\work\_CalcProp.htm]

File Edit View Advanced Window Help

Model Validation  
 Derivative Test  
 Phase Diagrams  
 Not available in this version  
 Property Calculation  
 Make Property Calculation

Setup Regression Utility

Temperature	=	303.15 K
Pressure	=	1.0000 Atm
Feed is stable		
<b>Name</b>	<b>Feed</b>	<b>Liquid</b>
ISOPENTANE	0.167816	0.167816
2-METHYLPENTANE	0.053641	0.053641
2-METHYLHEXANE	0.080587	0.080587
2,2,4-TRIMETHYLPENTANE	0.154405	0.154405
n-NONANE	0.107407	0.107407
n-DECANE	0.067176	0.067176
n-DODECANE	0.040231	0.040231
ETHANOL	0.133475	0.133475
WATER	0.018047	0.018047

-> PT-Flash (multi-phase): No of iterations = 0

Done

Done

# Methodology

Step 1 Identify target properties and target values

Step 2 Identify properties model

Step 3 Identify the possible blend mixture

Step 4 Generate the possible blend candidates

Step 5 Validate the model

Using GAMS (General Algebraic Modeling System)

Property constraint:

$$HV = \sum x_i HV_i$$

$$ON = \sum x_i ON_i$$

$$\rho_{mix} = \sum x_i \rho_i$$

$$\nu_{mix} = \frac{1}{\rho_{mix}} \exp\left(\sum \nu_i \ln \eta_i\right)$$

Volume constraint

$$V_{gasoline} \geq 0.5$$

$$V_{ethanol} \leq 0.05$$

# Methodology

Step 1 Identify target properties and target values

Step 2 Identify properties model

Step 3 Identify the possible blend mixture

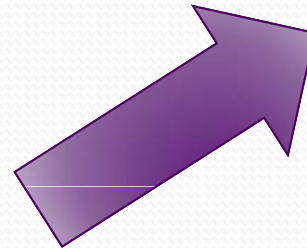
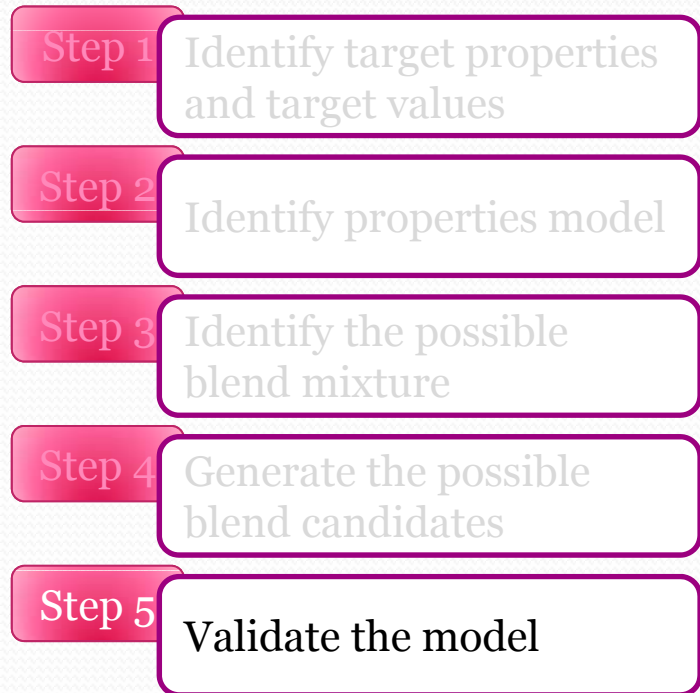
Step 4 Generate the possible blend candidates

Step 5 Validate the model

Target Properties	$\rho$ (kg/m <sup>3</sup> )	$\nu$ (mm <sup>2</sup> /s)	HHV (KJ/kg)	Wt % O <sub>2</sub>	ON
Gasoline	686.85	0.71	48028	0.00	95
Ethanol	769.84	1.84	29136	34.00	110
Butanol	805.89	3.15	36212	21.60	102.74
MTHF	808.20	0.36	36059	18.57	112.2



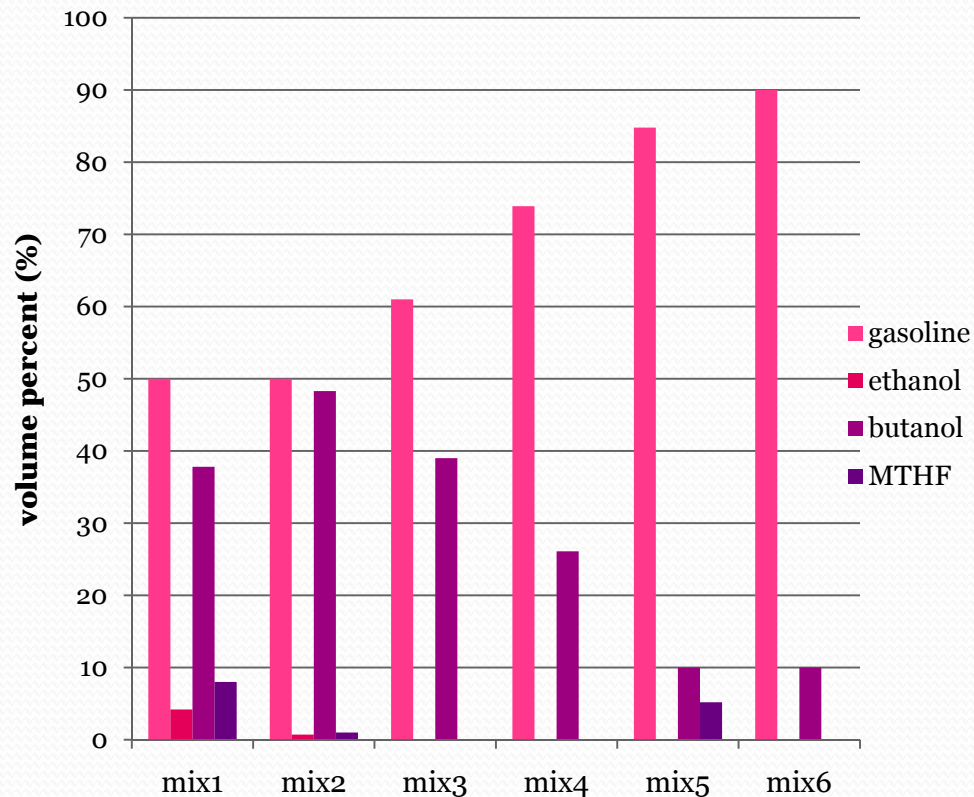
# Methodology



# Results

Composition	Mix 1	Mix2	Mix3	Mix4	Mix5	Mix6
Gasoline	0.500	0.500	0.610	0.739	0.848	0.90
Ethanol	0.042	0.007				
Butanol	0.378	0.483	0.390	0.261	0.100	0.10
MTHF	0.08	0.010			0.052	
<b>Property</b>						
HV	41.167	41.473	42.779	44.414	45.945	46.746
Density	749.156	749.130	736.186	720.522	707.696	700.000
Viscosity	0.00152	0.00174	0.0016	0.00138	0.00106	0.00109
ON	100	99	98	97	96	95

# Results



- All candidates consist of butanol
- Butanol is most favorable component due to attractive characteristics
- It has higher energy content which is close to gasoline energy content, less prone to water contamination and less corrosive

# Conclusion

- A systematic computer aided technique is a resources efficient technique which is suitable to find a set of target candidates
- Property model availability is one of the challenges in chemical product design

# Future work

- Including emission factor to produce a green fuel
- Model validation through a series of experimental work

# Acknowledgment

- CAPEC, Technical University of Denmark, Denmark
- Universiti Teknologi Malaysia, Malaysia.

A wide-angle photograph of a field of yellow rapeseed flowers. The flowers are in full bloom, creating a dense, textured sea of yellow. In the background, a flat horizon line separates the field from a clear, pale blue sky. The overall mood is bright and positive.

# THANK YOU

## Q&A session